Supporting Information: Experimental Details for:

"Columnar Discotic Liquid-crystalline Oxadiazoles as Electron-transport Materials"

Ya-Dong Zhang, Kim G. Jespersen, Michael Kempe, Julia A. Kornfield, Stephen Barlow, Bernard Kippelen, and Seth R. Marder

1a. Anhydrous K_2CO_3 (30 g) and methyl 3,4,5-trihydroxybenzoate (10 g, 5.4 mmol) was added to a deoxygenated mixture of DMF (100 mL) and of 1-bromooctane (35 g, 0.181 mol) under nitrogen. The mixture was heated at 80 ˚C for 6 h., when the reaction was judged complete by TLC analysis. The reaction mixture was cooled to room temperature, water (500 mL) was added, and the product was extracted with diethyl ether. The combined organic extracts were washed with water and dried over $MgSO_4$. After filtration, the solvent was evaporated under reduced pressure, and the crude product was passed through a column of silica gel using 2% ethyl acetate in hexane as eluent to afford **1a** as a yellow liquid (26 g, 5.0 mmol, 93%). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.25 (s, 2H, H_{arom}), 4.01 (m, 6H, 3 × OCH_2), 3.89 (s, 3H, OCH_3), 1.81 (m, 4H, 2 × CH_2), 1.73 (m, 2H, CH_2), 1.47 (m, 6H, 3 × CH_2), 1.28 (m, 24H, 12 × CH_2), 0.89 (t, 9H, 3 × CH_3. ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz) δ 166.90, 152.76, 142.27, 124.60, 107.88, 73.45, 69.10, 52.07, 31.87, 31.81, 30.30, 29.48, 29.31, 29.27, 26.04, 26.02, 22.68, 22.65, 14.06. GC/MS *m/z* 520 (M^+), 408 ($M^+ – C_8H_{17}$), 296 ($M^+ – C_8H_{17} – C_8H_{17}$), 184 ($M^+ – C_8H_{17} – C_8H_{17} – C_8H_{17}$). The data were in accordance with those given in a previous report of **1a**.[12]

2a. A solution of **1a** (10.0 g, 19.2 mmol) and excess hydrazine monohydrate in ethanol (180 mL) and heated to 80 ˚C for 32 h. Water (100 mL) was added and resulting precipitate was collected, dried under vacuum, and recrystallized from ethanol/water to yield pure 2a as a white solid (9.2 g, 17.9 mmol

92%). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.24 (br s, 1H, CON*H*), 6.93 (s, 2H, H_{arom}), 4.07 (br s, 2H, NH_2), 4.00 (m, 6H, 3 × OCH_2), 1.81 (m, 4H, 2 × CH_2), 1.73 (m, 2H, CH_2), 1.46 (m, 6H, 3 × CH_2), 1.29 (m, 24H, 12 × CH_2), 0.89 (t, 9H, 3 × CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz) δ 168.71, 153.17, 141.34, 127.41, 105.38, 73.49, 69.27, 31.86, 31.79, 30.27, 29.48, 29.31, 29.28, 29.25, 26.03, 22.65, 14.08 ppm. GC/MS *m/z* 520 (M^+), 489 ($M^+ - NHNH_2$), 377 ($M^+ - NHNH_2 - C_8H_{17}$). Anal. Calcd for $C_{31}H_{56}N_2O_4$: C, 71.49; H, 10.84; N, 5.38. Found: C, 71.23; H, 10.97; N, 5.43.

3a and **4a.** A solution of **2a** (6.00 g, 11.5 mmol) and 1,3,5-benzenetricarbonyl trichloride (1.00 g, 3.77 mmol) in THF (30 mL) was stirred at 0 ˚C for 1 h and at room temperature for 11 h; pyridine (3.0 mL) was added after 20 min the reaction mixture was poured into water (200 mL). The resulting precipitate of crude 3a (6.2 g) was collected and dried, and used without further characterization or purification in the preparation of **4a**. A solution of the crude **3a** (5.00 g, 2.91 mmol) in $POCl_3$ (40 mL) was heated to 80 ˚C for 16 h. Excess $POCl_3$ was removed by distillation and the residue was slowly added to ice-water and extracted with dichloromethane. After removal of solvent under reduced pressure, the crude product was purified by column chromatography on silica gel, using toluene/ethyl acetate (9:1) as eluent, followed by recrystallization from hexane/acetone to give 4a as a yellow solid (1.4 g, 0.84 mmol, 28%). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 9.07 (s, 3 H_{arom}), 7.40 (s, 6 H_{arom}), 4.14 (t, 12H, 6 × OCH_2), 4.08 (t, 6H, 3 × OCH_2), 1.89 (m, 12H, 6 × CH_2), 1.79 (m, 6H, 3 × CH_2), 1.59 (m, 18H, 9 × CH_2), 1.31 (m, 72H, 36 × CH_2), 0.90 (t, 27H, 9 × CH_2). ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz) δ 165.8, 162.7, 153.7, 141.8, 126.2, 117.8, 112.7, 105.6, 73.6, 69.5, 31.8, 29.4, 29.3, 26.1, 22.6, 14.1 ppm. FAB HRMS calcd for $C_{102}H_{162}N_6O_{12}$ $(M+H)^+$ 1664.2329. Found 1664.2324. Anal. Calcd for $C_{102}H_{162}N_6O_{12}$: C, 73.61; H, 9.81; N, 5.05. Found: C, 73.95; H, 9.96; N, 5.28.

Mobility measurements. Cells for mobility measurements were prepared from ITO (indium tin oxide) coated glass slides. Their thickness was controlled with calibrated spacers with a diameter of 20 μm. The material was placed at the edge of an opening of the empty cell and heated to 225 °C on a hot stage, and the melted material filled the cell by capillary action. Then a metallic weight heated to the same temperature was placed on top off the cells and heating was switched off, letting the samples cool down slowly to room temperature. The electron mobility was measured in air using the conventional time-of-flight method[20] with the samples mounted inside a temperature-controlled unit. A low-noise high-voltage power supply was used for applying the bias voltage. The photocurrent generated by irradiation with 6 ns pulses from a N_2 laser (337 nm) was amplified using a low-noise preamplifier and monitored with a digital oscilloscope. In order to keep $RC_p << t_t$ (transit time), resistance values were $R = 10^2 – 10^4\,\Omega$. C_p represents the total capacitance of the electrical circuit. Sample capacitance values were on the order of 10 pF. Neutral density filters were used when necessary to avoid excess charge accumulation in the samples.